Penalised regression models

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Overview

Penalised regression

- Ridge regression
- Lasso
- Elastic net
- Tuning the different parameters

Examples in R and applications

The linear model

$$y = \alpha + x\beta + \epsilon$$

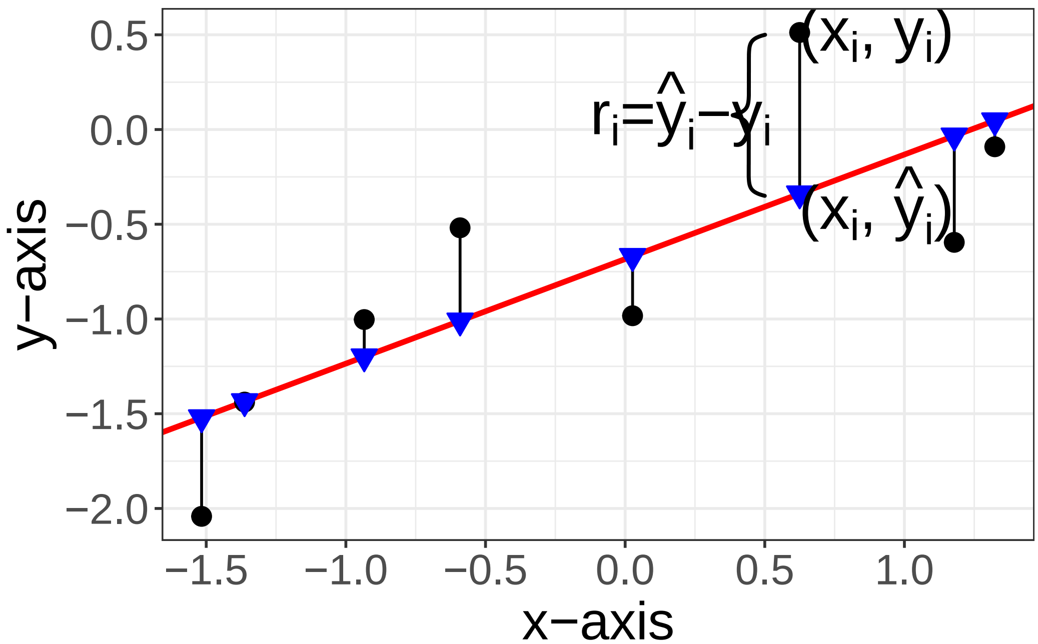
- y: Outcome, response, dependent variable with dimension: $n \times 1$
- x: Regressors, exposures, covariates, input, explanatory, or independent variables with dimension: $n \times p$
- ϵ: Residuals, error
- α: Intercept
- β: Regression coefficients, vector of length p

Classical regression

- The ordinary least squares $\hat{\beta}_{OLS}$ is defined as: $\hat{\beta}_{OLS} = \underbrace{(x^t x)^{(-1)}}_{p \times p} \underbrace{x^t}_{p \times n} \underbrace{y}_{n \times 1}$
- The residual sum of squares (RSS) is minimised by the ordinary least squares estimate:

$$
\begin{aligned}
RSS(\alpha, \beta) &= \epsilon_1^2 + ... + \epsilon_i^2 + ... + \epsilon_n^2 = \sum_{i=1}^{n} \epsilon_i^2 \\
&= \sum_{i=1}^{n} (y_i - \hat{y}_i)^2 = \sum_{i=1}^{n} (y_i - (\alpha + \beta x_i))^2
\end{aligned}
$$

Residual sum of squares (RSS)



- Note $\sum_{i=1}^{n} \epsilon_i = 0$

Classical regression and high-dimensional data

- When $n << p$ the ordinary least squares cannot be computed because $\underbrace{(x^t x)}_{p \times p}$ is singular (rank n)

Bias-variance trade-off

- The ordinary least squares estimate is best linear unbiased estimator (BLUE).
- BEST (smallest variance) among UNBIASED (zero bias) estimators.
- When considering high-dimensional data, the OLS estimate has a high variability. (dramatically different over different samples).
- We rather prefer an estimate that is biased (towards a sensible option, e.g. the Null), but is precise, (ie has low variance).

Idea

> Tip
>
> Control the estimates' variance by not allowing the to be too big. Constraints on how big they get. Does it remind you anything?

Motivation for penalised least squares

Minimise RSS but with penalty

$$\underset{\alpha,\beta}{argmin} = \underbrace{RSS(\alpha,\beta)}_{\text{Residual Sum of Squares}} + \underbrace{\lambda f(\beta)}_{\text{penalty}}$$

- Residual Sum of Squares: $RSS(\alpha,\beta) = \sum_{i=1}^{n} \left(y_i - (\alpha + \beta x_i)\right)^2$
- Penalty term as a function of the regression coefficients β: $f(\beta)$
- Regularization parameter: λ
- The intercept is not penalised

Motivation for penalised least squares

The penalty introduces a bias, so why do it?

- Which variables do we include? Only those for which it is worth to take the penalty.
- Occam's razor: It induces sparsity and favours models with lower complexity (Lasso and elastic net).
- Regularizes the inversion of $x^t x$ (Ridge regression).

Different penalty terms define different methods

$$\underset{\alpha,\beta}{argmin} = RSS(\alpha,\beta) + \lambda f(\beta)$$

- Ridge regression: L2 penalty: $\lambda f(\beta) = \lambda \sum_{j=1}^{p} \beta_j^2$
- Lasso regression: L1 penalty: $f(\beta) = \lambda \sum_{j=1}^{p} |\beta_j|$
- Elastic net regression: L1 + L2 penalty:

$$\lambda f(\beta) = \lambda_1 \sum_{j=1}^{p} |\beta_j| + \lambda_2 \sum_{j=1}^{p} \beta_j^2$$

Ridge regression

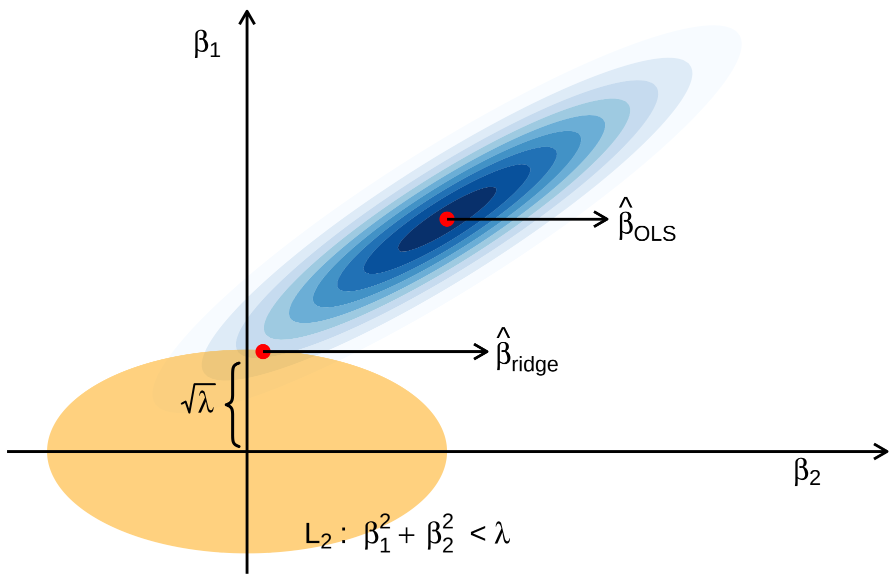
Ridge regression uses the L2 norm as penalty:

$$\underset{\alpha,\hat{\beta}_{Ridge}}{argmin} = \underbrace{RSS(\alpha,\beta)}_{\text{Residual Sum of Squares}} + \underbrace{\lambda \sum_{j=1}^{p} \beta_j^2}_{\text{penalty}}$$

Interpretation:

- The Ridge regression coefficient $\hat{\beta}_{Ridge}$ is a biased estimate, but has a reduced variance compared to $\hat{\beta}_{OLS}$.
- There is no intrinsic model selection in Ridge regression, all p variables will have $\hat{\beta}_{Ridge} \neq 0$.
- Minimise the RSS while forcing β not to be very large.

Ridge regression: Geometric interpretation



Ridge regression

$$\sum(Y_i - \alpha - \beta_1 x_i - \dots)^2 \text{ subject to } ||\beta||_2^2 \leq c^2$$

$$F(\alpha, \beta, \lambda) = \sum(Y_i - \alpha - \beta_1 x_i - \dots)^2 + \lambda(\beta_1^2 + \beta_2^2 + \dots - c^2)$$

How can we solve it?

- Partial derivatives
- Numerical solution using different values for λ. Note $\lambda \geq 0$:$argmin\{F(\alpha, \beta, \lambda)\} = RSS(\alpha, \beta) + \lambda \sum_{j=1}^{p} \beta_j^2$

When λ: $\lambda = 0$, then OLS, when $\lambda >> 0$, then β=0

Ridge regression and OLS

The ridge regression estimate is available in closed form

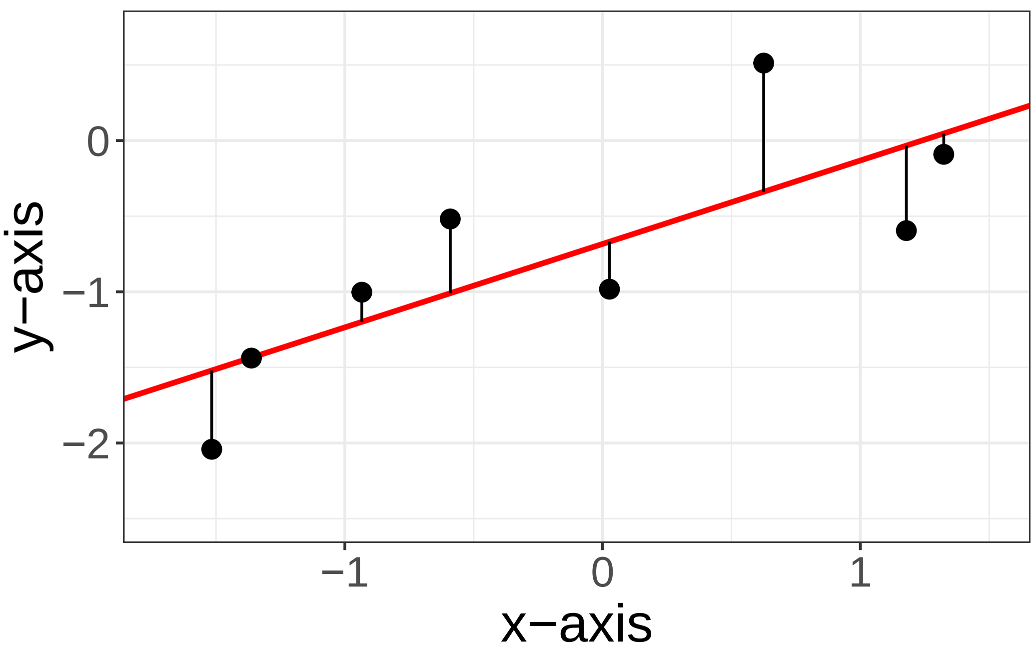
$$\hat{\beta}_{Ridge} = \underbrace{(x^t x + \lambda I)^{(-1)}}_{p \times p} \underbrace{x^t}_{p \times n} \underbrace{y}_{n \times 1}$$

where I is a $p \times p$ diagonal matrix with ones on the diagonal and zero on the off-diagonal

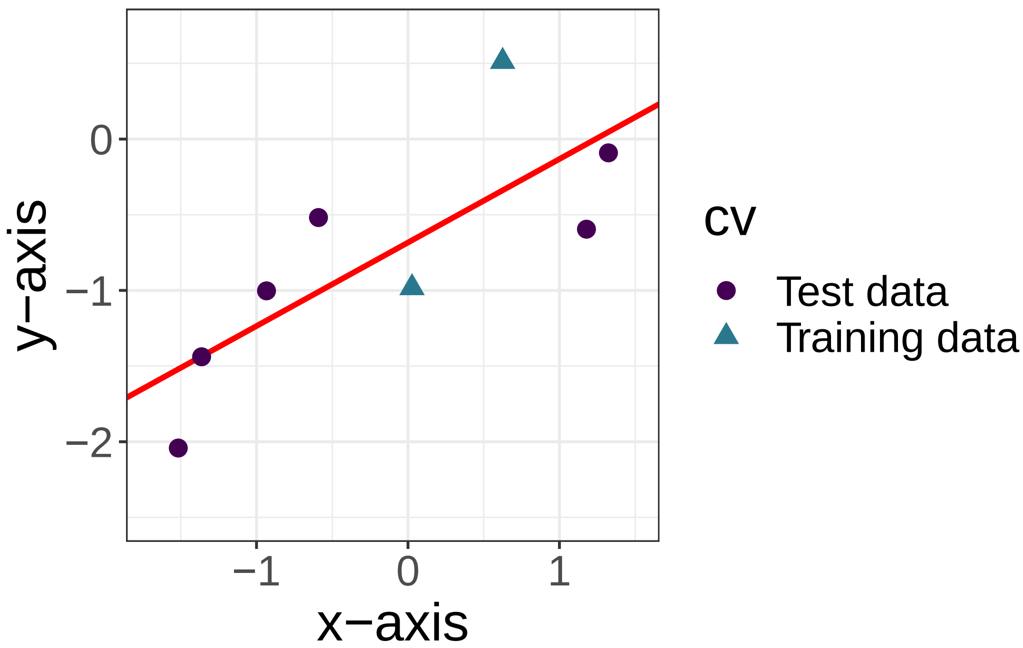
$$x^t x + \lambda I = n \begin{bmatrix} cov(x_1) & cov(x_{12}) & cov(x_{13}) \\ cov(x_{21}) & cov(x_2) & cov(x_{23}) \\ cov(x_{31}) & cov(x_{23}) & cov(x_3) \end{bmatrix} + \begin{bmatrix} \lambda & 0 & 0 \\ 0 & \lambda & 0 \\ 0 & 0 & \lambda \end{bmatrix}$$

This resembles the OLS estimate apart from $+\lambda I$.

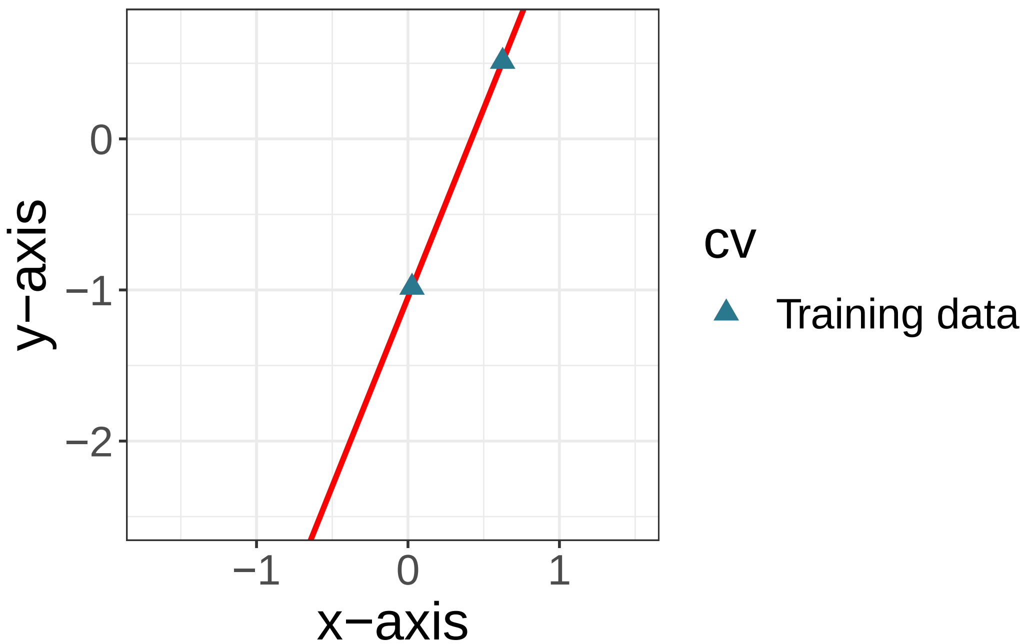
Ridge regression and OLS



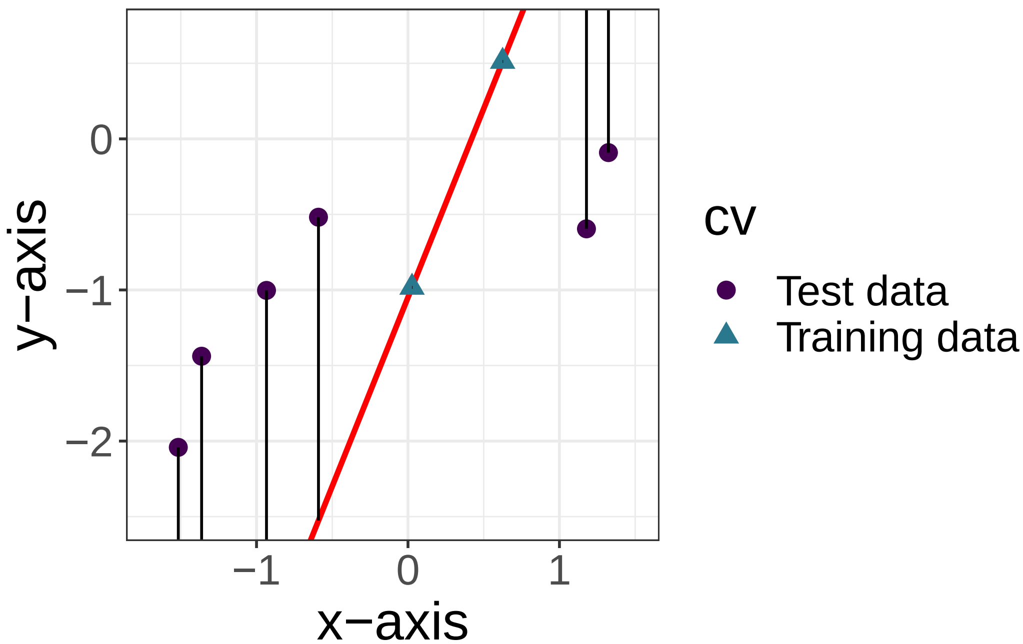
Ridge regression and OLS



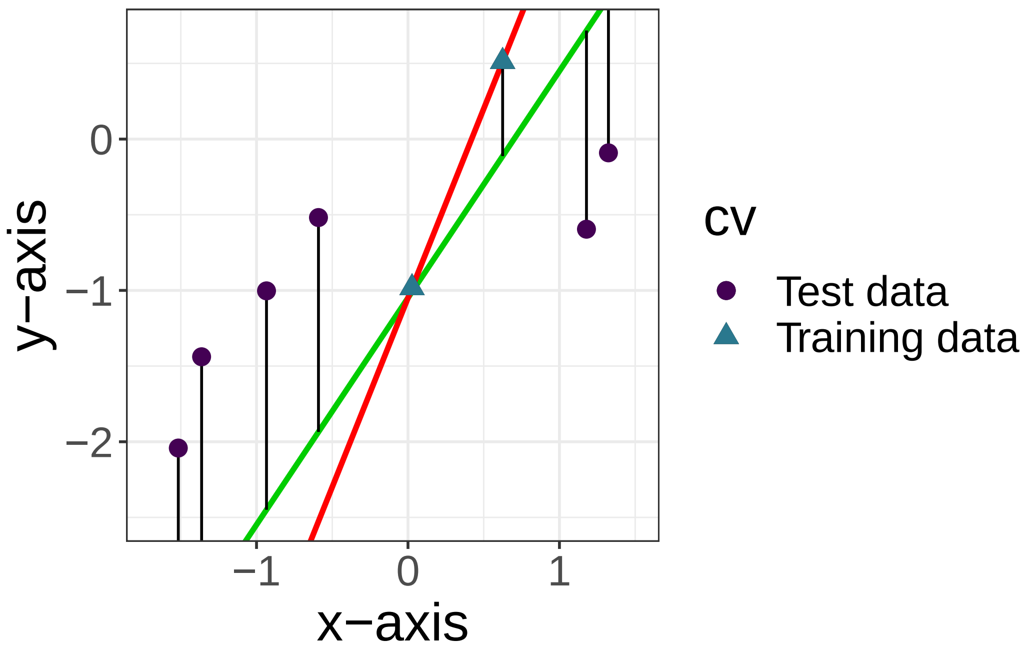
Ridge regression and OLS



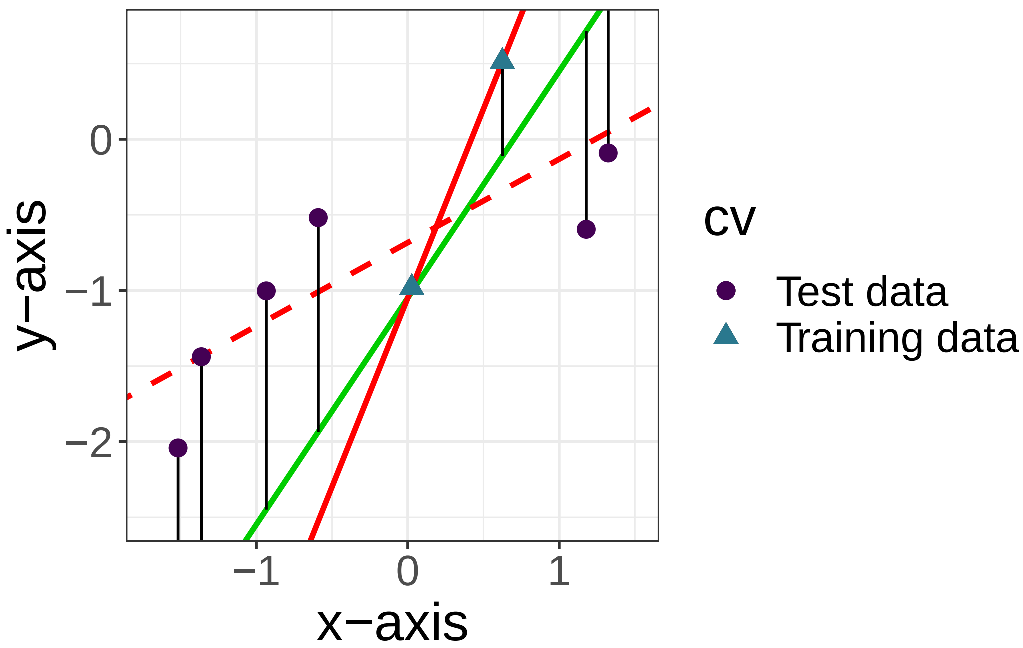
Ridge regression and OLS



Ridge regression and OLS



Ridge regression and OLS



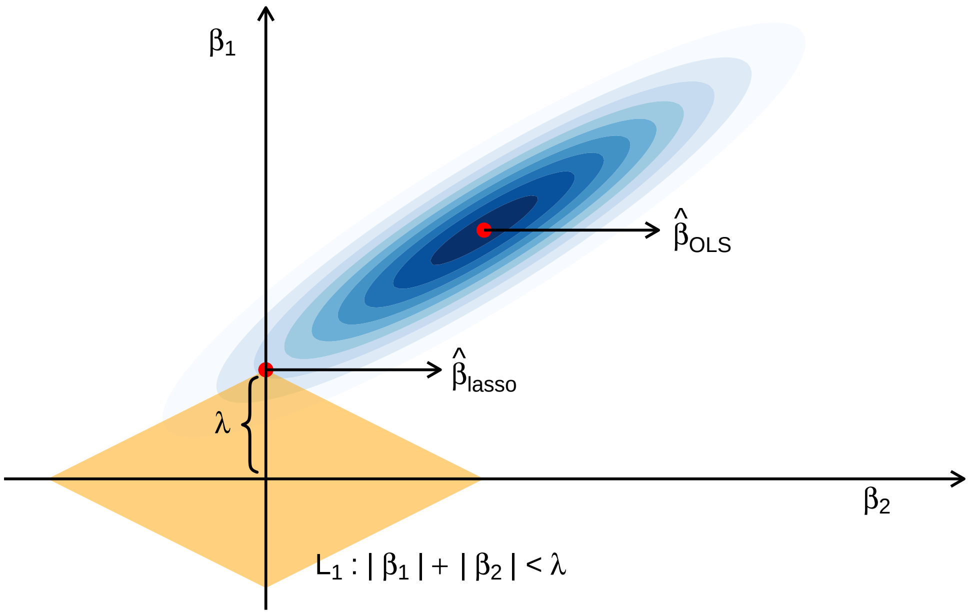
Lasso regression

$$\underset{\hat{\alpha},\hat{\beta}_{Lasso}}{argmin} = \underbrace{RSS(\alpha, \beta)}_{\text{Residual Sum of Squares}} + \underbrace{\lambda \sum_{j=1}^{p} |\beta_j|}_{\text{penalty}}$$

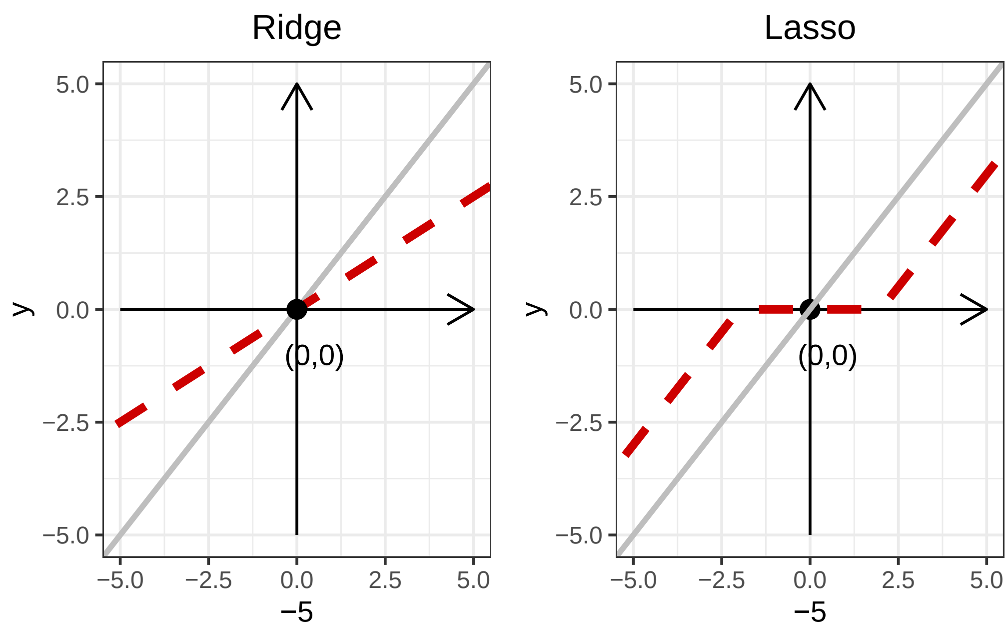
Interpretation:

- The Lasso regression coefficient $\hat{\beta}_{Lasso}$ is a biased estimate, but has a reduced variance compared to $\hat{\beta}_{OLS}$.
- There is an intrinsic model selection in Lasso regression, as it sets certain variables exactly to $\hat{\beta}_{Lasso} = 0$, and thus excludes them from the model.
- When two variables are highly correlated, Lasso includes only one (at random) and not both.

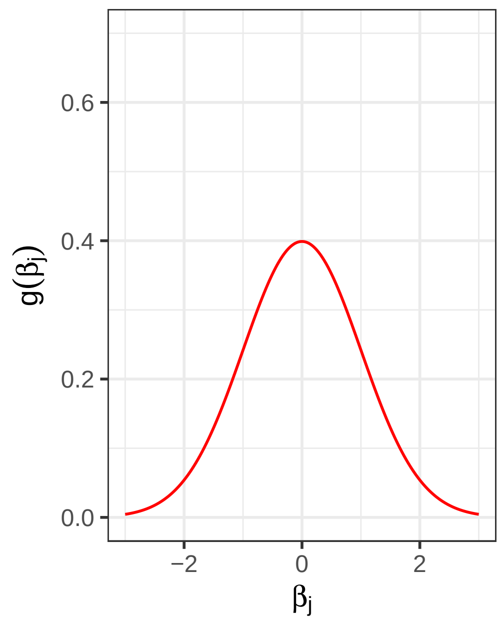
Lasso regression: Geometric interpretation

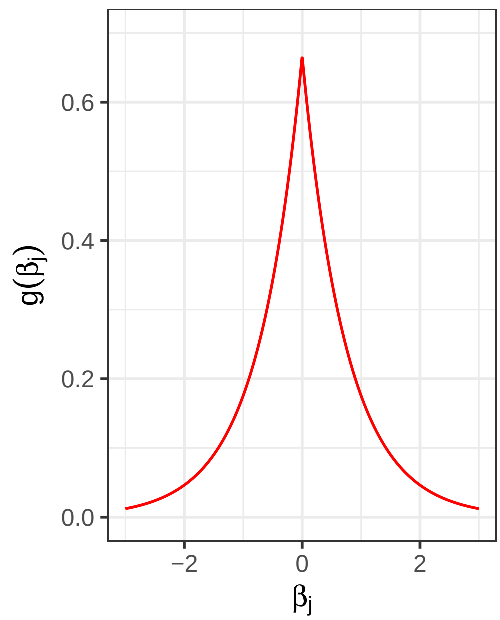


Ridge and lasso: Induced shrinkage



Ridge and lasso: Bayesian interpretation





Elastic net

$$\underset{\hat{\alpha},\hat{\beta}_{\text{Elastic net}}}{argmin} = \underbrace{RSS(\alpha,\beta)}_{\text{Residual Sum of Squares}} + \underbrace{\lambda_1 \sum_{j=1}^{p} |\beta_j| + \lambda_2 \sum_{j=1}^{p} \beta_j^2}_{\text{penalty}}$$

- The Elastic net regression coefficient $\hat{\beta}_{\text{Elastic net}}$ is a biased estimate, but has a reduced variance compared to $\hat{\beta}_{OLS}$
- There is an intrinsic model selection in Lasso regression, as it sets certain variables exactly to $\hat{\beta}_{\text{Elastic net}} = 0$, and thus excludes them from the model.
- When two variables are highly correlated, Elastic net includes both (Grouping property).

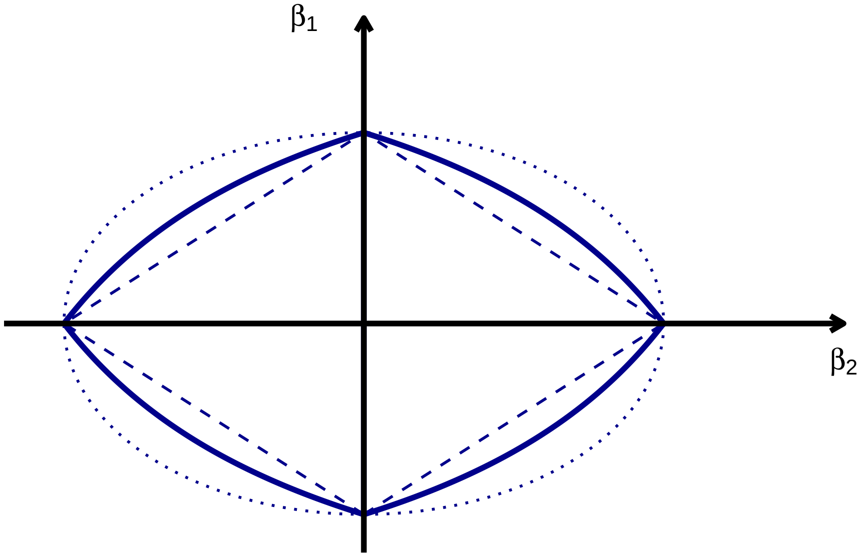
Elastic net regression: reparametrization

$$\underset{\hat{\alpha},\hat{\beta}_{\text{Elastic net}}}{argmin} = \underbrace{RSS(\alpha,\beta)}_{\text{Residual Sum of Squares}} + \lambda\left[\alpha\,||\beta||_1 + (1-\alpha)\,||\beta||_2^2\right]$$

- α can be seen as a mixing parameter
- When $\alpha = 0$ ridge regression

- When $\alpha = 1$ lasso regression
- How can we select the optimal λ and α?

Elastic net: Geometric interpretation



How to tune the regularisation parameter?

$$\underset{\alpha,\beta}{argmin} = RSS(\alpha, \beta) + \lambda f(\beta)$$

λ is the regularisation parameter

- $\lambda = 0$: No regularisation
- Small λ: Minimal regularisation
- Large λ: Strong regularisation
- How to choose the optimal λ?
- **Cross-validation**

Prediction using penalised regression

- Regularized regression is an ideal tool for prediction.
- We can define a prediction rule $\hat{f}(x)$ using the penalised regression coefficients:

$$\hat{y} = \hat{f}(x) = \alpha + x\hat{\beta}_{\text{Penalised}}$$

  where $\hat{\beta}_{\text{Penalised}}$ are the p regularized coefficients.

- Since Lasso and Elastic net force some $\hat{\beta}_{\text{Penalised}}$ to zero, variables with $\hat{\beta}_{\text{Penalised}} = 0$ are excluded from the model and do not contribute to the prediction rule.
- In contrast in Ridge regression variables contribute to $\hat{f}(x)$.

Penalised regression in R: `glmnet()`

```
glmnet(x, y, family, alpha,
  nlambda = 100,
  lambda.min.ratio = ifelse(nobs < nvars, 0.01, 0.0001),
  lambda = NULL, standardize = TRUE, intercept = TRUE
)
```

Input

- y: Outcome or response
- x: Predictors, formatted `as.matrix(x)`

Generalised linear models included

- family = `gaussian`, `binomial`, `poisson`, `multinomial`, `cox`, `mgaussian`

Penalised regression in R: `glmnet()`

```
glmnet(x, y, family,
  alpha,
  nlambda = 100, lambda.min.ratio = ifelse(nobs < nvars, 0.01, 0.0001), lambda = NULL,
  standardize = TRUE, intercept = TRUE
)
```

Penalised regression models

- Ridge regression: alpha = 0
- Lasso regression: alpha = 1
- Elastic net: 0 < alpha < 1

Regularisation parameter:

- Perform cross-validation

Penalised regression in R: `glmnet()`

```
glmnet.out <- glmnet(x, y, family, alpha)
```

Values:

- Intercept: `glmnet.out$a0`
- Regression coefficient estimates: `glmnet.out$beta`
- Regularisation parameters used: `glmnet.out$lambda`

Functions:

- Cross-validation: `cv.glmnet()`
- Regression coefficients: `coef(glmnet.out)`
- Prediction: `predict(glmnet.out, newx)`

Penalised regression in R: `glmnet()`

For more details on glmnet, see the useful vignette:

http://web.stanford.edu/~hastie/glmnet/glmnet_alpha.html

Other packages in R

- `lm.ridge` in the `MASS` package
- `lars` in the `lars` package
- `penalized` in the `penalized` package

Diabetes data

- y: quantitative measure of disease progression
- x: predictor matrix
    - clinical parameters: age, sex, bmi
    - map: blood pressure
    - tc: total cholesterol
    - ldl: low-density lipoprotein
    - hdl: high-density lipoprotein
    - tch: total cholesterol over hdl
    - ltg: triglycerides

Diabetes data

```r
library(lars)
library(dplyr)
library(glmnet)

data(diabetes)
x <- as.matrix(diabetes$x)
y <- diabetes$y

head(x)
```

```
              age         sex         bmi          map           tc         ldl
[1,]  0.038075906  0.05068012  0.06169621  0.021872355 -0.044223498 -0.03482076
[2,] -0.001882017 -0.04464164 -0.05147406 -0.026327835 -0.008448724 -0.01916334
[3,]  0.085298906  0.05068012  0.04445121 -0.005670611 -0.045599451 -0.03419447
[4,] -0.089062939 -0.04464164 -0.01159501 -0.036656447  0.012190569  0.02499059
[5,]  0.005383060 -0.04464164 -0.03638469  0.021872355  0.003934852  0.01559614
[6,] -0.092695478 -0.04464164 -0.04069594 -0.019442093 -0.068990650 -0.07928784
              hdl          tch          ltg          glu
[1,] -0.043400846 -0.002592262  0.019908421 -0.017646125
[2,]  0.074411564 -0.039493383 -0.068329744 -0.092204050
[3,] -0.032355932 -0.002592262  0.002863771 -0.025930339
[4,] -0.036037570  0.034308859  0.022692023 -0.009361911
[5,]  0.008142084 -0.002592262 -0.031991445 -0.046640874
[6,]  0.041276824 -0.076394504 -0.041180385 -0.096346157
```

Ridge regression and diabetes data

```r
library(lars)
library(dplyr)
library(glmnet)

data(diabetes)
x <- as.matrix(diabetes$x)
y <- diabetes$y
```

```r
cbind(
  lm(y ~ x) %>% coef(),
  glmnet(x, y, family = "gaussian", alpha = 0, lambda = 0.1) %>% coef(),
  glmnet(x, y, family = "gaussian", alpha = 0, lambda = 1) %>% coef()
)
```

```
11 x 3 sparse Matrix of class "dgCMatrix"
                                 s0          s0
(Intercept)  152.13348  152.133484  152.133484
age          -10.01220   -9.358965   -6.698824
sex         -239.81909 -238.769510 -233.325125
bmi          519.83979  520.713588  520.019917
map          324.39043  323.548886  319.639206
tc          -792.18416 -666.737488 -320.594626
ldl          476.74584  377.500940  103.343333
hdl          101.04457   45.579036 -104.230542
tch          177.06418  161.855769  124.122091
ltg          751.27932  703.885551  568.507179
glu           67.62539   68.277472   71.865726
```

Lasso regression and diabetes data

```r
cbind(
  lm(y ~ x) %>% coef(),
  glmnet(x, y, family = "gaussian", alpha = 1, lambda = 0.1) %>% coef(),
  glmnet(x, y, family = "gaussian", alpha = 1, lambda = 40) %>% coef()
)
```

```
11 x 3 sparse Matrix of class "dgCMatrix"
```

```
                                      s0          s0
(Intercept)  152.13348  152.133484 152.13348
age          -10.01220   -5.789635   .
sex         -239.81909 -234.457334   .
bmi          519.83979  522.819506  93.58588
map          324.39043  320.347881   .
tc          -792.18416 -534.397332   .
ldl          476.74584  271.305848   .
hdl          101.04457   -9.067565   .
tch          177.06418  146.255119   .
ltg          751.27932  655.715819  33.43273
glu           67.62539   66.410644   .
```

Elastic regression and diabetes data

```r
cbind(
  lm(y ~ x) %>% coef(),
  glmnet(x, y, family = "gaussian", alpha = 0.5, lambda = 0.1) %>% coef(),
  glmnet(x, y, family = "gaussian", alpha = 0.5, lambda = 40) %>% coef()
)
```

```
11 x 3 sparse Matrix of class "dgCMatrix"
                                      s0          s0
(Intercept)  152.13348  152.133484 152.13348
age          -10.01220   -7.373073   .
sex         -239.81909 -236.908421   .
bmi          519.83979  521.524719 308.42812
map          324.39043  321.784878  53.18902
tc          -792.18416 -570.166854   .
ldl          476.74584  302.943444   .
hdl          101.04457    .          .
tch          177.06418  144.752485   .
ltg          751.27932  669.554762 267.61977
glu           67.62539   67.483126   .
```

Example: Breast cancer data

- y: benign or aggressive tumor (binary)

Benign	Aggressive	Total
185	121	306

- x: gene expression of $p = 22,283$ genes
- $n = 306$: sample size
- Truly big data $n << p$

Breast cancer data and `glm()`

```
load("assets/JAMA2011_breast_cancer")

severity <- data_bc$rcb
x <- data_bc$x
```

```
glm.out <- glm(severity ~ as.matrix(x), family = "binomial")
glm.out$converged
```

Takes a lot of time and eventually you will get a warning that the algorithm did not converge!

Breast cancer data and lasso

```
lasso.out <- glmnet(x = as.matrix(x), y = severity,
                    family = "binomial", alpha = 1, lambda = 0.001)
sum(abs(lasso.out$beta) > 0)
```

```
[1] 288
```

```
lasso.out <- glmnet(x = as.matrix(x), y = severity,
                    family = "binomial", alpha = 1, lambda = 0.12)
sum(abs(lasso.out$beta) > 0)
```

```
[1] 6
```

```
lasso.out$a0
```

```
       s0
0.3236629
```

```r
lasso.out$beta %>% summary()
```

```
22283 x 1 sparse Matrix of class "dgCMatrix", with 6 entries
      i j            x
1  1662 1 -0.004526658
2  4752 1  0.058374857
3  9133 1 -0.009686168
4  9235 1  0.026345145
5 12416 1 -0.002190472
6 19988 1 -0.025081473
```

Breast cancer data and elastic net

```r
enet.out <- glmnet(x = as.matrix(x), y = severity,
                   family = "binomial", alpha = 0.5, lambda = 0.003)
sum(abs(enet.out$beta) > 0)
```

```
[1] 486
```

```r
enet.out <- glmnet(x = as.matrix(x), y = severity,
                   family = "binomial", alpha = 0.5, lambda = 0.26)
sum(abs(enet.out$beta) > 0)
```

```
[1] 6
```

```r
enet.out$a0
```

```
       s0
0.7666402
```

```r
enet.out$beta %>% summary()
```

```
22283 x 1 sparse Matrix of class "dgCMatrix", with 6 entries
      i j            x
1  1662 1 -0.007657373
2  4752 1  0.027947534
3  9133 1 -0.006866718
4  9235 1  0.007115454
5 12416 1 -0.001404657
6 19988 1 -0.014191285
```

Take away: Penalised regression models

- Regularized regression approaches minimise the residual sum of squares and an additional penalty function.
- Different penalties imply different approaches:
  - Ridge regression: $L2$
  - Lasso regression: $L1$
  - Elastic net regression: $L1 + L2$

Take away: Penalised regression models

- Penalized regression approaches are biased, they **underestimate** the size of the true effect.
- But they reduce the variance of the estimate and the prediction rule.
- Lasso and Elastic net perform an intrinsic model selection.
- The regularisation parameter λ can be chosen using cross-validation.

Questions?